

Experimental realization of a highly structured search algorithm

Xiwen Zhu, Ximing Fang, Mang Feng, Fei Du, Kelin Gao and Xi'an Mao

Laboratory of Magnetic Resonance and Atomic and Molecular Physics,

Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences,

Wuhan 430071, P. R. China

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Abstract

The highly structured search algorithm proposed by Hogg[Phys.Rev.Lett. 80,2473(1998)] is implemented experimentally for the 1-SAT problem in a single search step by using nuclear magnetic resonance technique with two-qubit sample. It is the first demonstration of the Hogg's algorithm, and can be readily extended to solving 1-SAT problem for more qubits in one step if the appropriate samples possessing more qubits are experimentally feasible.

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Quantum computers[1-5] can outperform classical ones owing to utilization of quantum mechanical effects. The potential for quantum parallel computing mainly resulted from superpositions and entanglements of quantum states has made quantum computers capable of solving classically intractable problems (such as factoring large integers[3]) and finding tractable solutions more rapidly(e. g., searching an unsorted database[6]). However, carrying out an actual quantum computing is much difficult although the rudiment of the quantum computing is easily understood and several quantum algorithm have been discovered. Among the approaches meeting the requirement for performing quantum computing, the nuclear magnetic resonance(NMR) technique[7,8] is considered to be one of current promising method, with which the Deutsch-Jozsa algorithm[9] and Grover's search one[6] has been experimentally implemented with two-qubit samples[10-13]. Recently, it was reported that an algorithmic benchmark has been experimentally realized using NMR with seven qubits[14]. It was easily found from those works that NMR can act as a considerably satisfactory small-scaled quantum computer to test the simple cases of the various quantum algorithm. In this contribution, also using NMR scheme with two-qubit sample, we report the first experimental demonstration of another quantum search algorithm. This algorithm, called a highly structured quantum search algorithm[15], was claimed to be much more efficient than Grover's algorithm[6] that ignores the problem structure, and can be exploited in many practical examples instead of for academic study alone as an artificial problem[9].

The Hogg's algorithm is associated with the combinatorial searching known as nondeterministic polynomial-time problems(NP)[16], an important class of intractable problems. Its prototype is the satisfiability problems(SAT)[16]. A SAT consists of a logic formula in n boolean variables, V_1, \dots, V_n , and the requirement to find an assignment, specifying a value for each binary variable, that makes the formula true. The logic formula can be expressed as a conjunction of m clauses and each clauses is a disjunction of some variables. When all the clauses have exactly k variables, the problem is called k -SAT, with 1-SAT being the simplest case. Combinatorial search aims at seeking the solution of a SAT from the total of 2^n assignments. In general, the computational cost of solving a SAT grows exponentially

with n in the worst case, making the SAT one of the most difficult NP problems[16]. For a few simple cases like 1-SAT and 2-SAT, however, solutions can be quickly and accurately determined without exponential cost using the regular structure of the problem. As each false clause for a given assignment is counted as a conflict, solutions are assignments with no conflicts. The classical search cost for such cases is $O(n)$ due to each clause eliminating one value for a single variable, but the quantum counterpart with Hogg's algorithm for 1-SAT and maximally constrained k-SAT a single step[15], with the help of quantum parallelism and interference combined with the problem structure, which shows very high efficiency for large n .

Actually, Hogg's algorithm consists of three stages[15]. First, one makes an equal superposition of bases, $|s\rangle$, of the n two-state quantum system as the initial state $|\psi_i\rangle = 2^{-\frac{n}{2}} \sum_s |s\rangle$, with bit strings s being all 2^n assignments of n variables. Secondly, a transformation R is applied on $|\psi_i\rangle$. The elements R_{ss} of the diagonal matrix R are determined by the conflicts c_s of s , which are governed by the constraints expressed in clauses of the logic formula. It is explicitly expressed as

$$R(s) = \begin{cases} \sqrt{2} \cos(2c - 1)\frac{\pi}{4} & \text{for even } m \\ i^c & \text{for odd } m. \end{cases} \quad (1)$$

Finally, an operation U with the form

$$U_{rs} = \begin{cases} 2^{-\frac{n-1}{2}} \cos[(n - m + 1 - 2d)\frac{\pi}{4}] & \text{for even } m \\ 2^{-\frac{n}{2}} e^{i(n-m)\frac{\pi}{4}} (-i)^d & \text{for odd } m, \end{cases}$$

is acted. It can be seen that the matrix elements U_{rs} depend only on the Hamming distance $d_{r,s}$ between r and s . As it describes the inconsistency of all the corresponding bits of bit strings r and s , $d_{r,s}$ has some correlation with conflicts c_s . By exploiting the intrinsic relation between $d_{r,s}$ and c_s and ingeniously constructing R_{ss} and U_{rs} with $d_{r,s}$ and c_s , making the combined transformation UR on $|\psi_i\rangle$ once is able to find the expected state, i. e., $UR|\psi_i\rangle = |\psi_0\rangle$, which has equal amplitudes among solutions and no amplitudes among nonsolutions.

In the view of quantum physics, Hogg's algorithm subtly makes use of the properties of quantum superposition and interference. When the calculating system is prepared on the equal superposition state, $|\psi_i\rangle = 2^{-\frac{n}{2}} \sum_s |s\rangle$, all the possible values, which can be assigned to the logical formula, regardless correct or incorrect, are embodied in the state. Then the state is subjected to the transform R , which gives a varied phase to each component state of the superposition state according to its conflicts c_s . The final operation U destructively annihilates every component state that its conflict is not zero, constructively enhances the correct component state that its conflicts is zero, finds out the exact component state that satisfies the logical formula. In one word, the essence of searching achieved in a single step is to examine all the assignments simultaneously and to make use of quantum interference embedded in UR. By a single step we mean the number of search steps or sequentially examined assignments, not the number of elementary computational operations required.

Our implementation of Hogg's algorithm was performed using solution NMR, applied to an ensemble of carbon-13 labelled chloroform molecules ($^{13}\text{CHCl}_3$). Two heteronuclear spins ^1H and ^{13}C in $^{13}\text{CHCl}_3$ work as two qubits in our quantum computing. Similar to other experiments[9-12,14,17-19] of quantum information processing using NMR, all the logic operations were realized by a specified sequence of radio-frequency (RF) pulses and the spin-spin coupling between the nuclei, and should be finished in the period of time much shorter than the relaxation times T_1 and T_2 of the nuclei in order to minimize the decoherence effect.

A quantum circuit for achieving this highly structured search in a two-qubit system is shown in Fig. 1. The algorithm starts in the state $|\psi_s\rangle = |00\rangle$, labelling the states of ^1H and ^{13}C spins from left to right respectively. As the state of a bulk sample at room temperature is described by a density matrix ρ_{th} for a thermally equilibrated system, we prepared an effective pure state $\rho = |00\rangle\langle 00|$ by temporal averaging[20], with which a deviation density matrix with diagonal elements of $\text{diag}(\rho_s)=[1,0,0,0]$ could be extracted from the summation over cyclic permutations of the populations of the $|01\rangle$, $|10\rangle$, and $|11\rangle$ states three times on the thermal matrix ρ_{th} . The Hadamard gates H in Fig. 1 were

implemented by using RF pulse sequence $\left(\frac{\pi}{2}\right)_y (\pi)_x$ or its equivalents and thus a uniform superposition state denoted by the density matrix $\rho_i = |\psi_i\rangle\langle\psi_i|$ with $\text{diag}(\rho_i)=[1,1,1,1]$ was obtained. Then two crucial operations R and U were applied, which are related to the problem structure and expressions for the logic formula and lead to the enhancement of solution states and the cancel of nonsolution states.

For our two-qubit system(i. e., $n = 2$), m , the number of clauses in the 1-SAT formula with satisfiable solutions can be assumed 2 or 1. When $m = 3$ and 4, no satisfying assignment exists due to over-constrained formula being unsatisfiable. Four satisfiable formulas in the $m = 2$ case are $V_1 \wedge V_2$, $V_1 \wedge \bar{V}_2$, $\bar{V}_1 \wedge V_2$ and $\bar{V}_1 \wedge \bar{V}_2$, where \bar{V}_i ($i = 1, 2$) are the negation of V_i . The corresponding solutions are easily found to be $|11\rangle$, $|10\rangle$, $|01\rangle$ and $|00\rangle$ respectively, where the logic variable with subscript 1 corresponds to the high qubit and 2 the low qubit. Similarly, the formulas for $m=1$ are V_2 , V_1 , \bar{V}_2 and \bar{V}_1 , corresponding to the unnormalized answer states $|01\rangle + |11\rangle$, $|10\rangle + |11\rangle$, $|00\rangle + |10\rangle$ and $|00\rangle + |01\rangle$, respectively. According to the number of states in the solutions, they can be called as single- and multiple- item searching. The algorithm on two instances of 1-SAT was experimentally demonstrated: one for $m = 2$ with clauses V_1 and V_2 , and the other for $m = 1$ with clause V_2 .

First of all, we have to derived the expressions for R and U from Ref.[15]. With Eq.(1), after calculating the conflicts c of each string assigned to the logical formula respectively, the elements of the diagonal matrices $R_{V_1 \wedge V_2}$ and R_{V_2} were calculated to be $\text{diag}(R_{V_1 \wedge V_2}) = [-1, 1, 1, 1]$ and $\text{diag}(R_{V_2}) = [i, 1, i, 1]$. U could be represented by $W\Gamma W$, where $W = H_1 \otimes H_2$ with H_i being the Hadamard gates, and Γ is a diagonal matrix with the diagonal elements

$$\Gamma_{rr} = \begin{cases} \sqrt{2} \cos[(m - 2|r| - 1)\frac{\pi}{4}] & \text{for even } m \\ i^{|r|} e^{-im\frac{\pi}{4}} & \text{for odd } m. \end{cases}$$

Elements of the diagonal matrices Γ for $m = 2$ and $m = 1$ were evaluated respectively as $\text{diag}(\Gamma_{m=2}) = [1, 1, 1, -1]$ and $\text{diag}(\Gamma_{m=1}) = [1, i, i, -1]$.

In order to realize the transformations with NMR, we designed the following RF pulse

sequences respectively:

$$\begin{aligned}
R_{V_1 \wedge V_2}: & \left(\frac{\pi}{2}\right)_{y_1} \left(\frac{\pi}{2}\right)_{x_1} \left(\frac{\pi}{2}\right)_{-y_1} - \frac{1}{2J} - \left(\frac{\pi}{2}\right)_{y_2} \left(\frac{\pi}{2}\right)_{x_2} \left(\frac{\pi}{2}\right)_{-y_2} \\
R_{V_2}: & \left(\frac{\pi}{2}\right)_{y_1} \left(\frac{\pi}{2}\right)_{x_1} \left(\frac{\pi}{2}\right)_{-y_1} \\
\Gamma_{m=2}: & \left(\frac{\pi}{2}\right)_{y_1} \left(\frac{\pi}{2}\right)_{-x_1} \left(\frac{\pi}{2}\right)_{-y_1} - \frac{1}{2J} - \left(\frac{\pi}{2}\right)_{y_2} \left(\frac{\pi}{2}\right)_{-x_2} \left(\frac{\pi}{2}\right)_{-y_2} \\
\Gamma_{m=1}: & \left(\frac{\pi}{2}\right)_{y_1} \left(\frac{\pi}{2}\right)_{x_1} \left(\frac{\pi}{2}\right)_{y_1} \left(\frac{\pi}{2}\right)_{y_2} \left(\frac{\pi}{2}\right)_{-x_2} \left(\frac{\pi}{2}\right)_{-y_2}
\end{aligned}$$

To make the best use of the available coherence time and to diminish errors due to the increased number of RF pulses, we finally optimized or reduced the pulse sequence constructed from the executing pulses of H, Γ and R mentioned above with the help of NMR principle[21]. The reduced pulse sequence for $(UR)_{V_1 \wedge V_2}$ and $(UR)_{V_2}$ shown in Fig. 2 were applied upon ρ_i , resulting the output matrix $\rho_0 \equiv |\psi_0\rangle\langle\psi_0| = (UR)\rho_i(UR)^\dagger$.

In order to read out the results of Hogg's algorithm accurately, a method of quantum state tomography[22] was adopted to reconstruct all the elements of the output density matrix ρ_0 . For this end, we applied different read-out pulses immediately after the searching pulses UR, one for each run. Explicitly, nine pulses $E_1 E_2$, $E_1 \left(\frac{\pi}{2}\right)_{x_2}$, $E_1 \left(\frac{\pi}{2}\right)_{y_2}$, $\left(\frac{\pi}{2}\right)_{x_1} E_2$, $\left(\frac{\pi}{2}\right)_{x_1} \left(\frac{\pi}{2}\right)_{x_2}$, $\left(\frac{\pi}{2}\right)_{x_1} \left(\frac{\pi}{2}\right)_{y_2}$, $\left(\frac{\pi}{2}\right)_{y_1} E_2$, $\left(\frac{\pi}{2}\right)_{y_1} \left(\frac{\pi}{2}\right)_{x_2}$ and $\left(\frac{\pi}{2}\right)_{y_1} \left(\frac{\pi}{2}\right)_{y_2}$ were exploited, where E_i ($i = 1, 2$) means no pulse acted on the i -th spin. Then we calculated the signal intensities by integrating the proton and carbon spectral lines acquired in each run and reproduced the whole matrix ρ_0 using the least-square fitting to the coupled equations connecting the signal intensities with the matrix elements. The recovered matrices ρ_0 from the experimental data were depicted in Fig. 3, along with the theoretical ones for comparison. It is clearly seen from Fig. 3 that only the elements of $\langle 11|\rho_0(V_1 \wedge V_2)|11\rangle$, $\langle 01|\rho_0(V_2)|01\rangle$, $\langle 01|\rho_0(V_2)|11\rangle$, $\langle 11|\rho_0(V_2)|01\rangle$ and $\langle 11|\rho_0(V_2)|11\rangle$ are significant, which justifies the searched items to be $|11\rangle$ for $V_1 \wedge V_2$ and unnormalized $|01\rangle + |11\rangle$ for V_2 formula. Due to experimental errors, however, several elements that should be zero theoretically still have small amounts of modulus, with the maxima being 8% for single-item and 19% for multiple-item searching.

Errors in the experiments result from several sources. The effective pure state $|00\rangle$ prepared by temporal averaging is generally not ideal, and small residual populations in the states $|01\rangle$, $|10\rangle$ and $|11\rangle$ of the deviation density matrix will surely cause errors in the

later stage of experiments. The inhomogeneity of RF fields and static magnetic fields and imperfections of the pulse-length calibration are also important sources of errors. Although we have tried to minimize these effects by careful adjustments of and measurements with the apparatus, some factors were still not well under control. Lastly but not insignificantly, losses of the coherence and populations of the density matrices in the whole process of experiments will lead to deviations of measured data from those expected by theory, especially for the off-diagonal elements. Perhaps that is why the maximum error in the multiple-item searching is larger than that in the single-item case. In all senses, minimizing experimental errors in all available ways is essential to accurately operating NMR quantum computers.

We have experimentally demonstrated a quantum algorithm for the highly structured combinatorial searching and found solutions to the 1-SAT problem in one algorithmic step almost surely using an NMR quantum computer with 2 qubits. By contrasting with other search methods that ignore the problem structure requiring $O(2^n)$ steps classically and $O(2^{\frac{n}{2}})$ steps on quantum computers[6], the searching with Hogg's algorithm can be accomplished in principle more efficiently. However, there is no difference between Hogg's algorithm and Grover's one when only two qubits are considered. The potential of the high efficiency owned by Hogg's algorithm will be displayed in solving various 1-SAT problems for $n > 2$ qubits in one step with current NMR technique, which can be readily extended from the present experiment, if the appropriate samples possessing more qubits can be experimentally feasible. Furthermore, Hogg's algorithm for 1-SAT could be generalized to the maximally constrained k-SAT problems[15], which have practical examples such as scheduling, finding low energy states of spin glasses and proteins, and automatic theorem proving. While scaling up an NMR computer to much large systems poses daunting challenges, building such a device with a few qubits by some creative approaches for demonstrating algorithms stated above and the others is promising.

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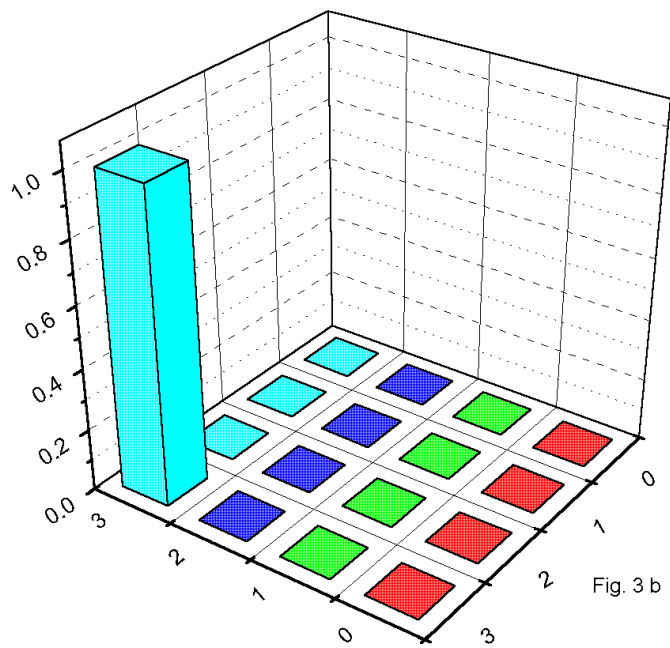
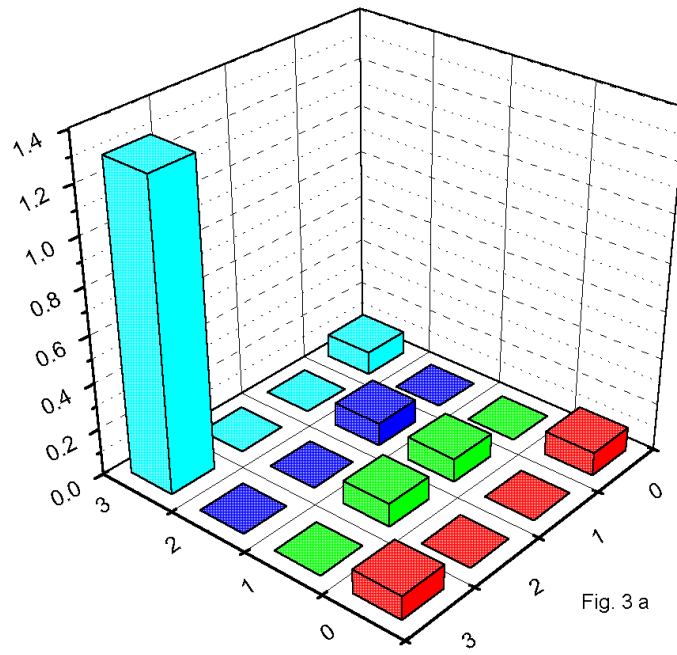
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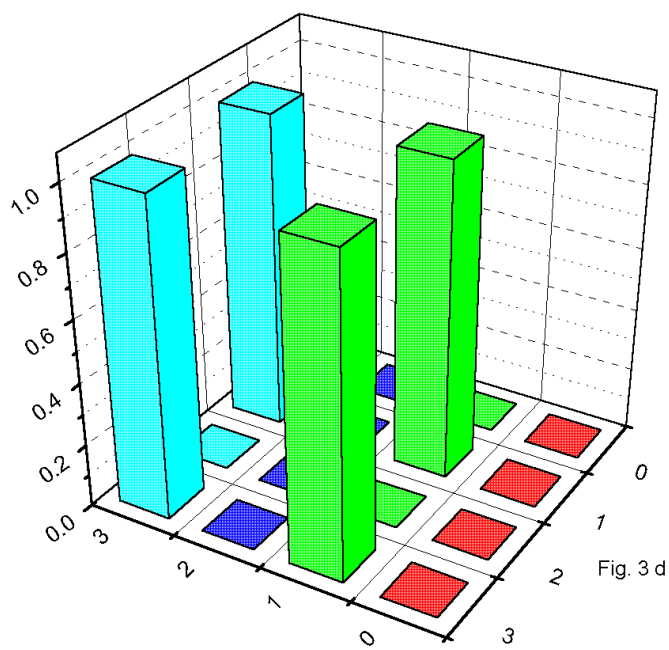
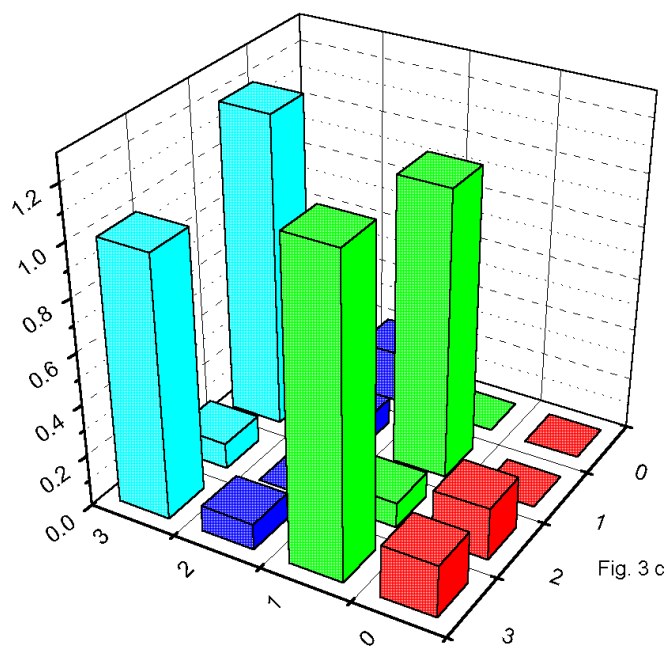
Captions of the figures

Figure 1 A quantum circuit for implementing a highly structure search algorithm on a two-qubit computer. Two Hadamard gates $H \otimes H$ transform an effective pure states $|\psi_s\rangle = |00\rangle$ into a uniform superposition state $|\psi_i\rangle$, which is then transformed to the answer state $|\psi_0\rangle$ after the action of gates R and U. For the definition of R and U, see text.

Figure 2 The reduced NMR pulse sequences used to execute a) $(UR)_{V_1 \wedge V_2}$ and b) $(UR)_{V_2}$ operations. Narrow and wide boxes correspond to $\frac{\pi}{2}$ and π pulses respectively. X and Y denote the pulses along the x- and y-axis, \overline{X} and \overline{Y} , opposite to the x- and y-axis. The time period τ is set equal to $\frac{1}{4J}$, where J is the size of the spin-spin coupling between nuclei 1H and ^{13}C . Experiments were performed using a Bruker ARX500 spectrometer. ^{13}C -labelled $CHCl_3$ were obtained from Cambridge Isotope Laboratories.

Figure 3 Experimentally recovered and theoretically expected deviation density matrices, ρ_0 , after completion of the combinatorial search with the aim of satisfying logic formulas of both $V_1 \wedge V_2$ and V_2 . The ordinate represents the modulus of matrix elements of ρ_0 (not normalized). The numbers 0, 1, 2 and 3 in the horizontal plane denote the subscripts $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$ of the elements, respectively. a) Experiment for $V_1 \wedge V_2$, b) Theory for $V_1 \wedge V_2$, c) Experiment for V_2 and d) Theory for V_2 .





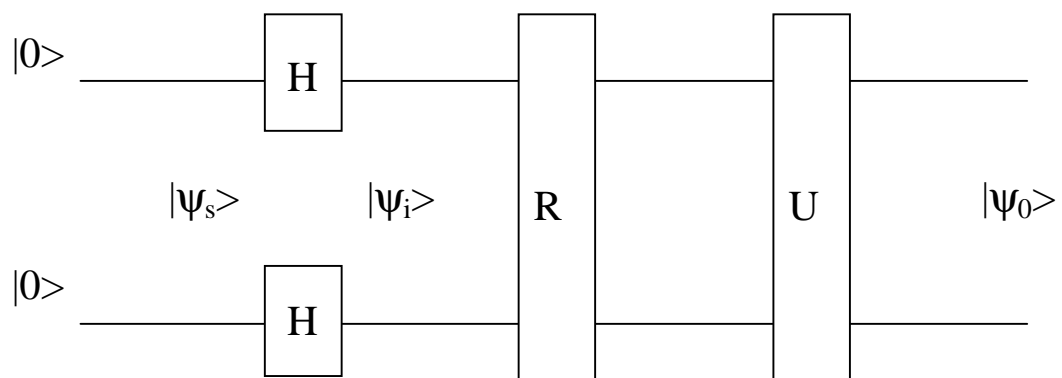


Fig. 1

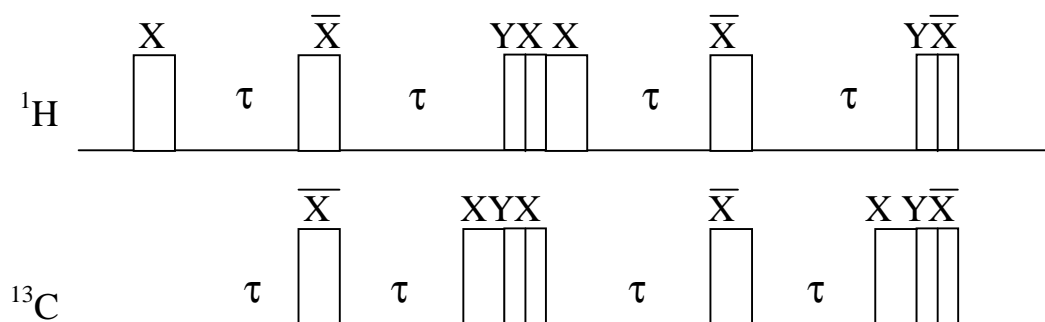


Fig. 2 a

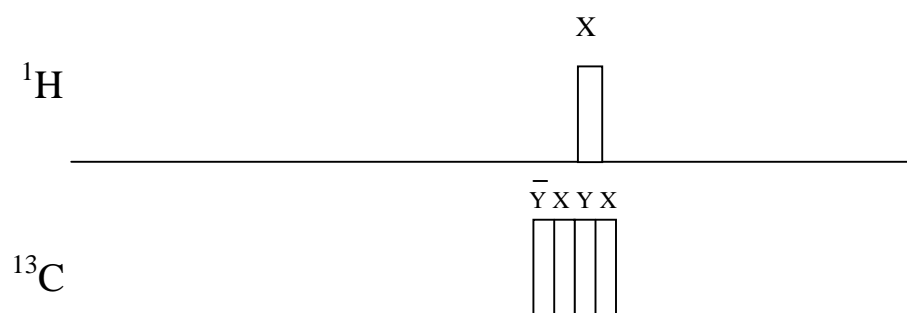


Fig. 2 b